

2,3,4,9-tetrahydro-1h-carbazol-3-ylacetonitrile
40496-58-0 | DTXSID60300275

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 337 °C

Global applicability domain: Inside

Local applicability domain index: 3.32e-01

Confidence level: 5.42e-01

Nearest Neighbors from the Training Set

Image not found

4-Nitrosodiphenylamine

Measured: 292

Predicted: 325

Image not found

4,4'-Methylenedianiline

Measured: 398

Predicted: 368

Image not found

4,4'-Oxydianiline

Measured: 350

Predicted: 363

Image not found

1,2-Benzenediamine,N-phenyl-

Measured: 313

Predicted: 363

Image not found

N-Phenyl-1,4-benzenediamine

Measured: 354

Predicted: 363